INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. X, 1093–1096 (1976)

Author Index, Volume X

Aiken, J.: See Aldrich, H. S.

Aldrich, H. S., Aiken, J., and Cusachs, L. C.: Radial Moment Analysis of Isovalent Hybridization in N_2, 955

Altmann, W.: See Kleindienst, H.

Ang, Y. A.: See Lo, B. W. N.

Banerjee, A. and Grein, F.: Convergence Behavior of Some Multiconfiguration Methods, 123

Bartlett, R. J. and Silver, D. M.: Correlation Energy in LiH, BH, HF with Many-Body Perturbation Theory Using Slater-Type Atomic Orbitals, 185

Baumgarten, E.: See Kleindienst, H.

Beebe, N. H. F.: On the Symmetry of Filled Shells, 1007

Behling, R., Bongers, A., and Küpper, T.: Upper and Lower Bounds to Critical Values of the Hartree Operator, 985

Bendazzoli, G. L., Orlandi, G., and Palmieri, P.: Spin-Orbit Coupling in Aromatic Hydrocarbons: A Semiempirical Evaluation on the Radiative Lifetimes of Naphthalene and Anthracene, 659

Beretta, E., Vetrano, F., and Solimano, F.: Some Remarks on a Double Perturbation Theory for Molecular Complexes, 175

Berthier, G.: See Meunier, A.

Besson, M. A. and Suard, M.: Analysis of the Space Correlation Factors in a MCSC Representation of LiH and Li_2 Molecules, 151

Bongers, A.: See Behling, R.

Brown, W. B.: See Whitton, W. M.

Bulski, M.: See Jaziorski, B.

Butler, P. H.: Calculation of *j* and *jm* Symbols for Arbitrary Compact Groups. II. An Alternate Procedure for Angular Momentum, 599

—— and Wybourne, B. G.: Calculation of *j* and *jm* Symbols for Arbitrary Compact Groups. I. Methodology, 581

—— and ——: Calculation of *j* and *jm* Symbols for Arbitrary Compact Groups. III. Application to $SO_3 \supset T \supset C_3 \supset C_1$, 615

Cadioli, B.: See Lazzeretti, P.

Cartling, B. G. and Whitmore, D. M.: Relativistic Molecular Spinors by Generalized Multiple Scattering Theory, 393

Cohen, M.: See Leopold, J. G.

Collins, M. P. S., Duke, B. J., Eilers, J. E., and O'Leary, B.: The Simulated *ab initio* Molecular Orbital Technique. VI. Open-Shell Radicals in the Spin Restricted Formalism, 629

Combs, L. L. and Miller, C. P.: The Use of Single Exponential Orbitals in One-Center Molecular Orbital Calculations, 455

Cusachs, L. C.: See Aldrich, H. S.

Davison, S. G. and Foo, E. N.: Energy Bands of *sp*-Hybrid Crystals in the Many-Neighbor Approximation, 867

Deal, W. J. and Young, R. H.: Perturbation Theory with an Approximate Perturbation: The Effect of Charge Overlap on Interatomic Interactions, 419

Delgado-Barrio, G.: See Smeyers, Y. G.

Duke, B. J.: See Collins, M. P. S.

Eilers, J. E.: See Collins, M. P. S.

Espinoza, L. L.: See Trsic, M.

Fimple, W. R. and Unwin, M. J.: A Finite-Difference Approach to the Electron Correlation Problem, 643

Fišer, J.: See Vojtík, J.

Foo, E. N.: See Davison, S. G.

Fusco, M. A.: See Garrod, C.

Garrod, C. and Fusco, M. A.: A Density Matrix Variational Calculation for Atomic Be, 495

George, J. K.: See Trindle, C.

Gianturco, F. A.: On the Scattering of Slow Protons by Diatomic Targets, 37

Goodisman, J.: Valence-Electron Theory Using the Thomas–Fermi–Dirac Model: Application to the K Atom and the K^- Ion, 341

Gopinathan, M. S.: On the Hypervirial Theorem and the Scaling Problem, 975

Grabenstetter, J. E., Tseng, T. J., and Grein, F.: Generation of Genealogical Spin Eigenfunctions, 143

Grein, F.: See Banerjee, A.

——: See Grabenstetter, J. E.

Guichon, P. A. M.: See Kibler, M. R.

Gunnarsson, O. and Johansson, P.: The Spin-

Density-Functional Formalism for Quantum Mechanical Calculations: Test on Diatomic Molecules with an Efficient Numerical Method, 307

Hagstrom, S. A.: See Sims, J. S.
Hameka, H. F. and Svendsen, E. N.: Errors in the Calculations of First-Order and Second-Order Energy Perturbations, 249
Hehenberger, M.: See McIntosh, H. V.
Hendeković, J.: Complex Molecular Orbital Method: Open-Shell Theory, 1025
Hyslop, J. and Rees, D.: An Iterative Scheme for Electronic Systems Using One-Electron Green's Functions, 569

Jafri, J. A. and Whitten, J. L.: Iterative Introduction of Integral Approximations with Error Bounds in SCF Calculations, 383
Jakubowski, P.: Best Optimized One-Electron Wave-Functions. I. The General Procedure of Optimization, 719
——: Best Optimized One-Electron Wave-Functions. II. Isoelectronic Series of Li, Be, B, and C, 733
——: Best Optimized One-Electron Wave-Functions. III. Direct Examination of Optimization Effectiveness, 739
——: Best Optimized One-Electron Wave-Functions. IV. Ionization Energies of Atoms, 743
Jankowski, K.: A Characterization of Pairs of Subspaces for Quantum Chemical Applications of the Galerkin–Petrov Method, 683
Jaziorski, B., Bulski, M., and Piela, L.: First-Order Perturbation Treatment of the Short-Range Repulsion in a System of Many Closed-Shell Atoms or Molecules, 281
Johannsson, P.: See Gunnarsson, O.
Julg, A. and Marinelli, F.: Halogénures Alcalins: Un Modèle Incluant une Délocalisation à Courte Distance Application à la Stabilité Relative des Divers Arrangements Cristallins, 1037
——: See Pellegatti, A.

Kaniauskas, J. M.: See Rudzikas, Z. B.
Kaplan, I. G. and Rodimova, O. B.: Group Theoretical Classification of States of a Molecular System at Definite States of Its Constituent Parts, 699
Kashiwagi, H.: Integral Approximations on the Basis of Semiorthogonalized Orbitals, 135
Katriel, J.: See Leopold, J. G.
——: See Moiseyev, N.
Kaufman, J. J. and Kerman, E.: Quantum Chemical Calculations of Thioridazine, 559
—— and Popkie, H. E.: Similarity in the Pattern per Atom-Pair in Benzene of Contributions to Total Energy or Total Overlap Populations, 543
——: See Popkie, H. E.
Kennard, E. B. and Waber, J. T.: Calculated Anisotropies in the Fermi Surface of Alkali Metals, 261
Kerman, E.: See Kaufman, J. J.
Kertész, M.: See Mayer, I.
Kibler, M. R. and Guichon, P. A. M.: Clebsch–Gordan Coefficients for Chains of Groups of Interest in Quantum Chemistry, 87
Kitaura, K. and Morokuma, K.: A New Energy Decomposition Scheme for Molecular Interactions within the Hartree–Fock Approximation, 325
Kleindienst, H. and Altmann, W.: I. Lineare Fehlerminimisierung Ein Verfahren zur Eigenwertverechnung bei Schrödinger-Operatoren, 873
——, Baumgarten, E., and Altmann, W.: II. Eigenwertberechnung beim Dreikorperproblem, 887
Klimo, V. and Tiňo, J.: Spin-Extended Hartree-Fock Calculation for Hydrocarbon π-Radicals, 761
Klymenko, V. E.: See Kuprievich, V. A.
Kothekar, V.: Molecular Orbital Interpretation of Isomer Shifts and Quadrupole Splitting of the Mössbauer γ-Line in the Compounds of Antimony and Tin, 993
Kotos, W.: Long- and Intermediate-Range Interaction in Three Lowest Sigma States of the HeH^+ Ion, 217
Kruglyak, Yu. A.: See Kryachko, E. S.
Kryachko, E. S. and Kruglyak, Yu. A.: On the Solution of the *N*-Completeness Problem, 937
Küpper, T.: See Behling, R.
Kuprievich, V. A. and Klymenko, V. E.: Computation Scheme for Optimizing Multiconfiguration Wave-Functions, 941

Lathouwers, L.: A New Approach to Canonical Orthonormalisation, 413
Lazzeretti, P., Cadioli, B., and Pincelli, U.: Calculations of Electric Dipole Polarizabilities of Polyatomic Molecules, 771
Leclerc, J. C.: Comparative Study of Unconventional 1*s* Basis Functions for the $^1\Sigma_g^+$ Ground State of H_2 and H_2^{++}, 439

——: Hybrid Slater-Gaussian-Type 1*s* Orbitals for the $^1\Sigma_g^+$ Ground State of H_2 and He_2^+, 781
Leopold, J. G., Cohen, M., and Katriel, J.: A Study of Löwdin's Criterion for Completeness of Basis Sets, 1049
Levy, B.: See Meunier, A.
Lim, T. K.: Exclusion Principle and the Symmetry Adapted Wave-Functions, 299
——: Many-Electron Theory in the Waller-Hartree Spin-Free Method, 791
Lo, B. W. N. and Ang, Y. A.: Calculations of the $G_n(a)$ Auxiliary Function in Gaussian Orbit-Orbit Integrals, 1087
Lochmann, R.: Crystal Calculation Using the PCILO Method, 901
—— and Weller, T.: Calculation of Interactions within the PCILO Framework, 909
Lohr, L. L., Jr.: Hybrid Orbitals and the Runge-Lenz Vector, 799
——: See Mohraz, M.

Marinelli, F.: See Julg, A.
Matsen, F. A.: Spin-Free Quantum Chemistry. XVII. The Hückel-Hubbard Theory and the Woodward-Hoffmann Rules, 511
——: Spin-Free Quantum Chemistry. XVIII. The Unitary Group Formulation of the Many-Electron Problem, 525
Matsuoka, O.: Molecular Integrals of Relativistic Effects with Gaussian-Type Orbitals, 379
Mayer, I. and Kertész, M.: A Comparison of Different DODS Methods When the Number of Electrons Increases, 961
McIntosh, H. V., Hehenberger, M., and Reyes-Sanchez, M.: Lattice Dynamics with Second Neighbor Interactions. II. Greens Formula, 191
Meunier, A., Levy, B., and Berthier, G.: The N^2 Problem in Molecular CI Calculations, 1061
Miller, C. P.: See Combs, L. L.
Mohammad, S. N.: See Sannigrahi, A. B.
Mohraz, M. and Lohr, L. L., Jr.: A Comparison of Orthogonalized Plane Wave and Augmented Plane Wave Methods for Calculating Photodetachment Cross-Sections, 811
Moiseyev, N. and Katriel, J.: Stability, Continuity, and Symmetry of Variational Wave-Functions, 1011
Morokuma, K.: See Kitaura, K.
Muftakhova, F. I.: On Calculation of Energy States of Polyatomic Molecules and Clusters in a Solid, 1077

Nakajima, T.: See Toyota, A.
Neely, S. C.: See Pilkington, P. W.
Nerbrant, P.-O.: The Use of Partitioning Technique in the Solution of Operator Equations for Ionizations and Excitations, 233
Novaro, O. and Yanez, F.: Gaussian-Type Bases for the Calculation of the Interaction Energy Between Neon Atoms, 545

O'Leary, B.: See Collins, M. P. S.
Olivier, G.: See Weislinger, E.
Orlandi, G.: See Bendazzoli, G. L.

Palmieri, P.: See Bendazzoli, G. L.
Pellegatti, A. and Julg, A.: Influence de la Structure de Diverses Fonctions sur l'Evaluation de l'Energie de Correlation, 113
Piela, L.: See Jaziorski, B.
Pilkington, P. W. and Neely, S. C.: Matrix Elements for an Approximate *ab initio* π-Electron Theory, 473
Pincelli, U.: See Lazzeretti, P.
Popkie, H. E. and Kaufman, J. J.: *Ab initio* LCAO-MO-SCF Calculations of Chlorpromazine and Promazine, 569
——: See Kaufman, J. J.

Ra, Ø.: Orthogonalization of Overlapping Orbitals by Optimal Polynomials. I. Polynomials Constructed from Spectral Radii, 5
——: Asymptotic Properties of Inverses of Cyclic Overlap Matrices in the Large Separation Limit, 57
Raimondi, M. and Simonetta, M.: The Orthogonality Problem in Valence Bond Calculations, 1057
Rees, D.: See Hyslop, J.
Reyes-Sanchez, R.: See McIntosh, H. V.
Ritchie, A. G.: Electronic Energies of the Hydrogen Molecule $D'\Pi_u$ and $B'\Sigma_u$ States, 1071
Rodimova, O. B.: See Kaplan, I. G.
Rudzikas, Z. B. and Kaniauskas, J. M.: Generalized Spherical Functions in the Theory of Many-Electron Atoms, 837
Rumble, J. R., Jr.: See Sims, J. S.

Sanhueza, J. E.: See Trsic, M.
Sannigrahi, A. B. and Mohammad, S. N.: On the Applicability of the Selected Valence Electron Split-Shell Model to Ionic Molecules, 181; Erratum, 715

Schulman, J. M.: Obituary: Reflections on the Scientific Career of Jeremy Musher, 1
Schurr, J. M.: Light Absorption at High Intensities. Comparison of Quantum Theory and Semi-Classical Results, 359
Sharma, R. R.: Evaluation of Two-Center Integrals Using α-Functions, 1075
Silver, D. M.: See Bartlett, R. J.
Simonetta, M.: See Raimondi, M.
Sims, J. S., Hagstrom, S. A., and Rumble, J. R., Jr.: Combined CI-HY Studies of Atomic States. IV. The Four Lowest ^1S and Four Lowest ^1P States of He and the Lowest ^1S and ^1P States of H^-, 853
Smeyers, Y. G. and Delgado-Barrio, G.: Analysis of the Half-Projected Hartree–Fock Function: Density Matrix, Natural Orbitals, and Configuration Interaction Equivalence, 461
Solimano, F.: See Beretta, E.
Suard, M.: See Besson, M. A.
Svendsen, E. N.: See Hameka, H. F.

Tanaka, T.: See Toyota, A.
Tatum, J. P.: Angular Correlation of Electrons in the Ground State of Helium, 967
Tiño, J: See Klimo, V.
Toyota, A., Tanaka, T., and Nakajima, T.: The Instabilities of the Hartree–Fock Solutions and the Lattice Instabilities for Conjugated Hydrocarbons: The Bond-Order and Bond-Length Alternations, 917
Trindle, C. and George, J. K.: Integral Hellman–Feynman Computations on H_3ABH_n—H_2ABH_{n+1} Rearrangements, 21
Trsic, M., Sanhueza, J. E., and Espinoza, L. L.: Singlet and Triplet Excited State Electric Dipole Polarizabilities of Conjugated Hydrocarbons, 429
Tseng, T. J.: See Grabenstetter, J. E.

Unwin, M. J.: See Fimple, W. R.

Vetrano, F.: See Beretta, E.
Viccaro, M. H. de A.: Symmetry Property of Lowdin's "alpha" Function, 1081
Vojtík, J. and Fišer, ˇ.: Time Reversal and Spin-Adapted Wave-Fu ctions, 1083

Waber, J. T.: See Kennard, E. B.
Weislinger, E. and Olivier, G.: Applications of a Quantum Virial Theorem to Kronig and Penney's Model and to a Diatomic Molecule in Static Approximation, 225
Weller, T.: See Lochmann, R.
Weltin, E. E.: Direct Minimization of the Energy by Simultaneous Variation of Parameters in Nonorthogonal Basis Functions. I. Method, 163
Whitmore, D. M.: See Cartling, B. G.
Whitten, J. L.: See Jafri, J. A.
Whitton, W. N. and Brown, W. B.: The Relationship Between the Rayleigh–Schrodinger and Asymptotic Perturbation Theories of Intermolecular Forces, 71
Witschel, W.: Generating Functions for Oscillator Matrix Elements, 951
Wójcik, M. J.: Theory of the Infrared Spectra of the Hydrogen Bond in Molecular Crystals, 747
Wybourne, B. G.: See Butler, P. H.

Yanez, F.: See Novaro, O.
Young, R. H.: See Deal, W. J.